Applicants: Albert C. Pierce et al.

Application No.: 10/790,507

In the Specification

Please delete previous Abstract at page 43 and add the following <u>new Abstract:</u>

Methods of identifying potential ligands for macromolecular targets are disclosed herein. The methods comprise providing models of three dimensional structural information for ligands or a ligand:macromolecule complex, mapping spatial relationships between the models, and identifying one or more pairs of matching bonds. Databases and apparatuses are also provided.